1 Flame-wall interactions of lean premixed flames under 2 elevated, rising pressure conditions

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11 Abstract

12 Direct numerical simulation (DNS) of laminar lean methane-air and *n*-
13 heptane-air premixed flames with high exhaust gas recirculation (EGR) ra-
14 tios propagating towards inert walls in a head-on quenching configuration
15 is conducted to investigate flame-wall interactions at relatively high initial
16 pressure conditions. This study considers the flame propagation under iso-
17 choric process after ignition while the piston is at top dead center (TDC). The
18 effects of EGR ratio, equivalence ratio, initial pressure and wall temperature
19 on heat loss and quenching distance are investigated. The results showed
20 that change of EGR ratio in fuel mixture significantly affects the maximum
21 wall heat flux and the heat flux induced by the burned gas temperature. The
22 normalized flame-wall interaction time is not influenced over a range of EGR
23 ratios, equivalence ratios and initial chamber pressures for methane-air and
24 *n*-heptane-air flames at fixed wall temperature conditions. The dimensional
25 flame-wall interaction time is almost constant when the chamber pressure is

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Preprint submitted to Fuel

October 17, 2016

doubled. The influence of low temperature oxidation in n -heptane flames on wall heat flux induced by temperature differences between the preheated fuel mixture and the wall is found to be insignificant. Moreover, both thermal conductivity near the wall and quenching distance are sensitive to the wall temperature, and have a substantial influence on the wall heat flux.

Keywords: Laminar Premixed Flames, Direct Numerical Simulation, Pressure Rising Process, Wall Heat Flux, Flame-wall Interactions

PACS: 47.15.-x, 47.27.ek, 47.70.Pq

1. Introduction

As emission regulations become more stringent, achieving both higher thermal efficiencies and reduced pollutant emissions is key to designing combustion devices. Recently, lean-boosted combustion with a high exhaust gas recirculation (EGR) level has been of particular interest for automotive engines, because both combustion efficiency and pollutant reduction are improved. The presence of diluted reactants further decreases the end-gas temperature and improves knock resistance [1, 2]. In addition, it was shown that the effective octane number can be increased by increasing the EGR ratio of the fuel mixtures [2]. However, heat loss characteristics are likely to be modified by such thermo-chemical conditions. Therefore, to achieve higher thermal efficiency by further reducing wall heat loss, it is important to understand heat transfer characteristics through the wall as well as the effects of relevant parameters such as EGR ratio γ , equivalence ratio ϕ , and wall temperature T_{wall} on these characteristics.

With improvements in computational technology, direct numerical simu-

50 lation (DNS) has become an important tool for investigating flame-wall in-
 51 teractions. Important quantities of flame-wall interaction phenomenon such
 52 as maximum wall heat flux and quenching distance have been extensively
 53 studied in previous numerical studies [3–8]. Interactions of laminar hydro-
 54 gen premixed flames with walls have been studied in a head-on quenching
 55 configuration using a one-dimensional DNS with detailed chemistry in Ref.
 56 [3, 4]. Dabireau et al. [3] have shown that at atmospheric pressure with
 57 inert boundary conditions, premixed flames generate high heat release rate
 58 near the wall than it does away from the wall. Owston et al. [4] investi-
 59 gated the effects of equivalence ratio and pressure on wall heat flux Φ_q , and
 60 the results show a significant increase in maximum Φ_q when the pressure
 61 is doubled. Owston et al. [5] have also investigated laminar *n*-heptane-air
 62 flames at different wall temperatures under constant pressure conditions.
 63 They have found a significant increase in the maximum Φ_q with increasing
 64 wall temperature from 300-1200 K in stoichiometric flames. A similar trend
 65 in maximum wall heat flux has also been reported using DNS of laminar
 66 stoichiometric methane, propane [6, 7] and iso-octane [8] premixed flames
 67 with wall temperature ranging from 300-600 K. Overall trends of quenching
 68 distance and the maximum Φ_q are similar in experimental studies [9, 10].
 69 A more detailed discussion of flame-wall interactions on DNS and experi-
 70 mental studies can be found in Ref. [11]. The aforementioned DNS studies
 71 on flame-wall interaction phenomenon consider constant pressure conditions.
 72 Whereas, in a constant volume vessel such as IC engines, the mean pressure
 73 increases during combustion which significantly influences wall heat transfer
 74 characteristics via temporal evolution of thermo-chemical properties. One

75 consequence is that flame thickness rapidly decreases with **increasing** pres-
76 sure, leading **to a decreased quenching distance** near the wall. **This** results
77 in an increased maximum wall heat flux [12]. Therefore, the mechanism
78 **influencing** overall wall heat flux is based on a complex balance of varying
79 flame properties due to **environmental changes** in the vessel as combustion
80 proceeds. **This** mechanism needs to be understood to lower the heat loss
81 for high-efficiency engines. In this study, due to the enormous computa-
82 tional resources required by DNS, **a** one-dimensional configuration similar to
83 the previous studies [3–8] is employed. **Moreover**, the compromise made in
84 the numerical configuration is accommodated **by** employing a more complex
85 chemistry, an isochoric process and relatively high pressure conditions. Thus,
86 the present results add new insight to our knowledge **of** flame–wall interac-
87 tion phenomena. This study also serves as a preliminary DNS for the future
88 three-dimensional DNS configuration which is similar to our previous DNS
89 studies [12, 13].

90 In this study, a series of one-dimensional DNS of lean methane–air and *n*-
91 heptane–air premixed flames with different EGR ratios propagating towards
92 inert walls in a head-on quenching configuration is conducted in a constant
93 volume vessel under elevated, rising pressure conditions to investigate the
94 effects of EGR ratio, equivalence ratio, initial pressure and wall temperature
95 on wall heat flux and quenching distance. This paper is organized as fol-
96 lows: The details of the DNS database is explained in Sec. 2, the results are
97 discussed in Sec. 3 and the conclusions are summarized in the final section.

98 2. Direct numerical simulation

99 The DNS code developed in our previous study [14] is employed. The
 100 fully-compressible governing equations for conservation of mass, momentum,
 101 energy and chemical species mass fractions, **respectively** can be written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + (\nabla \rho \mathbf{u} \mathbf{u}) = -\nabla \cdot \mathbf{P}, \quad (2)$$

$$\begin{aligned} \frac{\partial \rho T}{\partial t} + \nabla \cdot (\rho \mathbf{u} T) &= \frac{1}{\bar{c}_v} \nabla \cdot (\lambda \nabla T) - \frac{1}{\bar{c}_v} \sum_{i=1}^{N_s} (\rho Y_i \mathbf{V}_i c_{p,i} \nabla T) \\ &\quad - \frac{T}{\bar{c}_v} \sum_{i=1}^{N_s} [R_i \nabla \cdot (\rho Y_i \mathbf{V}_i)] - \frac{1}{\bar{c}_v} \mathbf{P} : (\nabla \mathbf{u}) \\ &\quad - \frac{1}{\bar{c}_v} \sum_{i=1}^{N_s} (h_i w_i) + \frac{T}{\bar{c}_v} \sum_{i=1}^{N_s} (R_i w_i), \end{aligned} \quad (3)$$

$$\frac{\partial Y_i}{\partial t} + \mathbf{u} \cdot \nabla Y_i = -\frac{1}{\rho} \nabla \cdot (\rho Y_i \mathbf{V}_i) + \frac{w_i}{\rho}. \quad (4)$$

105 where, ρ , $\mathbf{u}$, T , λ and N_s denote density, fluid velocity vector, temperature,
 106 thermal conductivity and the number of chemical species, respectively. Y_i ,
 107 $\mathbf{V}_i$, R_i , h_i , w_i , $c_{v,i}$ and $c_{p,i}$ denote, respectively, mass fraction, diffusion
 108 velocity, characteristic gas constant, enthalpy, reaction rate, specific heat
 109 capacities at constant volume and pressure for chemical species i . The stress
 110 tensor, $\mathbf{P}$ is given by

$$\mathbf{P} = \left[p + \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \right] \mathbf{I} - \mu \left[(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T \right], \quad (5)$$

111 where p , μ and $\mathbf{I}$ denote pressure, dynamic viscosity and the unit tensor,
 112 respectively. The mixture averaged specific heat capacity at constant volume,

113 $\bar{c}_v$ is given by

$$\bar{c}_v = \sum_{i=1}^{N_s} c_{v,i} Y_i \quad (6)$$

114 The Soret effect, the Dufour effect, pressure gradient diffusion, bulk viscosity
115 and radiative heat transfer are assumed to be negligible. The GRI-Mech 3.0
116 kinetic mechanism [15], which includes 53 reactive species and 325 elemen-
117 tary reactions, is used to describe methane–air combustion chemistry. For
118 *n*-heptane–air premixed flames, a reduced kinetic mechanism, which includes
119 37 reactive species and 61 elementary reactions is used [16]. Temperature
120 dependence of the viscosity, the thermal conductivity and the diffusion coef-
121 ficients are taken into account by linking the CHEMKIN-II packages [17, 18].
122 The governing equations are discretized using a fourth-order central finite dif-
123 ference scheme, and advanced in time by using the third order Runge-Kutta
124 method with $\Delta t = 1\text{ns}$. The fourth order compact finite difference filter [19]
125 is used to eliminate unphysical oscillations with higher spatial frequencies
126 than the spatial resolution. Only the reaction source terms are advanced
127 by the implicit method [20]. For the boundary condition, isothermal and
128 no-slip conditions expressed in the form of the Navier-Stokes characteristic
129 boundary condition (NSCBC) [21, 22] are imposed on both of the walls and
130 the wall surfaces are assumed to be chemically inert. The initial distribution
131 of species mass fraction is uniform.

132 The schematic of the computational domain **representing** the constant
133 volume vessel in the present study is shown in Fig. 1a. Figure 1b shows
134 the initial temperature distribution (T_{ini}) in the domain. The computational
135 domain has a closed configuration with walls at both ends and has a size
136 of $L_x = 5.0\text{ mm}$, which is discretized with uniform mesh, ensuring at least

80 grid points within the laminar flame thickness at the initial pressure to resolve the flame-wall interactions. This domain length represents the state when the piston head is at the top dead center (TDC) at the end of the compression stroke. Although this length is smaller than that in practical applications, the present domain length is chosen to allow flames to develop before impinging on the wall. T_{ini} is given as a Gaussian distribution and written as follows:

$$T_{ini} = T_{pre} + (T_{max} - T_{pre}) \exp\left(-\frac{r^2}{2\sigma_T^2}\right), \quad (7)$$

$$\sigma_T = r_c/3. \quad (8)$$

Here, T_{max} , T_{pre} , r_c , r and σ_T denote the maximum temperature of the ignition kernel, preheat temperature, radius of the ignition kernel, distance from center and the distance from center to position at which the temperature gradient is maximum, respectively.

Table 1 shows the relevant parameters of methane and n -heptane flames. γ indicates the EGR ratio. $S_{L,0}$, $\delta_{th,0}$ and $T_{ad,0}$ denote the laminar burning velocity, the laminar flame thickness based on the maximum temperature gradient, and the adiabatic flame temperature for initial flames, respectively. The subscript 0 indicates the quantity obtained from the laminar flame under constant initial pressure P_{ini} and T_{pre} conditions. In this study, T_{ini} , T_{max} , T_{pre} and r_c are the same for all cases. T_{max} is 1600 K, T_{pre} is 700 K and r_c is taken to be 0.5 mm. The present study simulates the phenomena at which the flame propagates under isochoric process after ignition while the piston is at TDC. After the mixture is ignited at the center of the domain, the flame propagates towards both ends. As the flame propagates, the pressure in the

domain increases and the effects of time-varying thermo-chemical properties can be addressed using the present DNS configuration. Since the initial preheated temperature is set to 700 K, the mean pressure (P_{mean}) is expected to increase by a factor of 2.4–2.7 for the present lean hydrocarbon flames. Both methane–air and n -heptane–air mixtures are diluted with EGR consisting of O₂, N₂, H₂O and CO₂. The mole fraction of H₂O in EGR is twice that of CO₂ in methane flames and 0.875 times that in n -heptane flames. The effects of EGR ratio, equivalence ratio, initial pressure and wall temperature on wall heat flux and quenching distance are discussed.

3. Results and discussions

3.1. Influence of EGR ratio, equivalence ratio and initial pressure

Figure 2 shows the temporal developments of the mean pressure of the domain as well as the maximum heat flux of methane–air flames for an equivalence ratio of 0.5 at different EGR ratios. Here, mean pressure is defined as pressure averaged in the whole domain. Wall heat flux is defined as the product of the thermal conductivity of the gas mixture and the temperature gradient on the wall, written as follows:

$$\Phi_q = -\lambda \nabla T|_{wall} \quad (9)$$

The wall temperature is fixed at 450 K. The time is normalized using the corresponding characteristic flame time ($\tau_{F,0} = \delta_{th,0}/S_{L,0}$). Therefore $\tau_{F,0}$ is different for each case, and can be calculated from Table 1. For this reason, the flame with the fastest laminar burning velocity (case M10W045) reaches the wall first, but has the largest non-dimensional time duration when

182 it impinges on the wall. Note that the heat flux induced by temperature
 183 differences between the preheated fuel mixture and the wall in the early
 184 period ($t/\tau_{F,0} < 1$) is high due to the initial developments of a temperature
 185 profile near the wall (i.e., the thermal boundary layer development in the
 186 2D and 3D fields.). The heat flux stabilizes after approximately $1\tau_{F,0}$ and
 187 has values around 0.1 MW/m^2 for all 3 cases. When the flame impinges
 188 on the wall, the wall heat flux at the attached point increases drastically.
 189 The maximum Φ_q decreases by 37% when the EGR ratio increase is 10%
 190 (M10W045 and M20W045). This is because the flame is thicker at higher
 191 EGR ratios. The wall heat flux induced by the burned gas is also reduced
 192 since the flame temperature is lower for higher EGR ratios.

193 Figure 3a shows the temporal developments of wall heat flux for flames
 194 with different equivalence ratios. The EGR ratio (γ), initial pressure and
 195 wall temperature are kept constant at 20%, 10 atm and 450 K, respectively.
 196 It was found that changing the equivalence ratio has a higher impact on
 197 the maximum wall heat flux than changing the EGR ratio. The maximum
 198 Φ_q is 83% higher for the increased ϕ case, ($\phi=0.6$, M20W045E), because a
 199 thinner flame can reach the wall closer thereby increasing the temperature
 200 gradient on the wall. Moreover, the heat flux induced by the burned gas
 201 temperature is also higher than that in M20W045 ($\phi=0.5$) since the flame
 202 temperature is higher. Although the time span of the maximum Φ_q acting on
 203 the wall is much shorter than that of the wall heat flux induced by burned
 204 gas temperature, it was shown that the wall heat flux induced by flame
 205 impingement (maximum wall heat flux) contributes substantially to the total
 206 heat loss during combustion [13].

207 The initial pressure is doubled to investigate pressure effects on flame-wall
 208 interactions. Figure 3b shows the temporal developments of mean pressure
 209 and maximum heat flux for different initial pressure cases, $P_{ini} = 10$ atm
 210 (M20W045) and $P_{ini} = 20$ atm (M20W045P). The maximum P_{mean} reaches
 211 up to 50 atm when the flame impingement occurs in M20W045P. Since the
 212 burning speed is slower in M20W045P, a longer time is required for the flame
 213 to reach the wall. However, the flame-wall interaction time τ_{fw} , which can
 214 be defined as the time required for Φ_q to reach its maximum from its half
 215 value [9], does not seem to be affected when the pressure is doubled. This
 216 result is consistent with an experimental study for stoichiometric methane
 217 flames under constant pressure conditions (0.5 - 17 atm) by Sotton et al. [23].
 218 Here, τ_{fw} is 1.93 ms and 1.91 ms for $P_{ini} = 10$ atm (M20W045) and $P_{ini} =$
 219 20 atm (M20W045P), respectively. In addition, regardless of any conditions
 220 reported in this study – different EGR ratios, equivalence ratios and initial
 221 pressures – the normalized τ_{fw} are similar when normalized by $\tau_{F,0}$, and they
 222 are in the range of 0.73-0.76 $\tau_{F,0}$. The maximum Φ_q of M20W045P is 43%
 223 higher than that of M20W045 due to a smaller quenching distance, which is
 224 discussed in Sec. 3.2.

225 3.2. Influence of wall temperature

226 The wall temperature of an engine cylinder has important effects on wall
 227 heat transfer. Thus, the influence of wall temperature on the wall heat flux
 228 is investigated in this section. The equivalence ratio, EGR ratio and initial
 229 pressure is fixed at 0.5, 20% and 10 atm, respectively. Both methane-air
 230 and *n*-heptane-air flames are considered since low-temperature chemistry of

231 *n*-heptane flames will be influenced by the wall temperature. Figure 4 shows
 232 the wall heat flux development at different wall temperature conditions. It
 233 should be noted that wall temperatures higher than 900 K was conducted
 234 for *n*-heptane flames as well, but only the results of $T_{wall} = 450 - 900\text{K}$ are
 235 shown since autoignition occurred near the hot wall region. Wall heat flux
 236 induced by the burned gas temperature decreases slightly due to the decrease
 237 in temperature difference between the wall and burned gas, when higher wall
 238 temperatures are considered. It should be noted that insensitivity of the τ_{fw}
 239 normalized by $\tau_{F,0}$, which is explained in Sec. 3.1, still holds for *n*-heptane
 240 flame at $T_{wall} = 450\text{K}$ and has a value of $0.77\tau_{F,0}$. Thus, this insensitivity
 241 is not influenced by the presence of two-stage ignition of large hydrocarbon
 242 flames.

243 The maximum Φ_q increases drastically with increasing wall tempera-
 244 ture, and the maximum Φ_q of *n*-heptane flames is comparable with those
 245 of methane flames. One of the contributions to this high wall heat flux can
 246 be explained by thermal conductivity of the gaseous mixture. Figure 5 shows
 247 the maximum Φ_q and thermal conductivity of the gaseous mixture on the
 248 wall as a function of wall temperature. Clearly, the maximum Φ_q has a pos-
 249 itive correlation with λ , suggesting that the effects of λ should be taken into
 250 account for prediction of heat loss through the wall. Another contribution
 251 can be explained by the near wall flame behavior. For higher T_{wall} cases,
 252 the unburned temperature of the reactant near the wall region increases due
 253 to heat transfer from the wall, resulting in higher flame speed and shorter
 254 quenching distance near the wall than that in the cold wall case. This phe-
 255 nomenon can be seen in Fig. 6, which shows the temporal development of

256 temperature profiles with respect to wall distance for methane and *n*-heptane
 257 flames. For the methane flame at $T_{wall} = 450\text{K}$ (M20W045), the flame speed
 258 decreases steadily as it propagates, then decreases drastically in the near
 259 wall region. For $T_{wall} = 900\text{K}$ (M20W090), the flame propagation speed in
 260 the near wall region is comparable to the speed away from the wall and the
 261 flame can approach the wall closer than it does in the cold wall case, thereby
 262 increasing the temperature gradient near the wall. Since heat loss is lower
 263 before flame impingement occurs for hot wall cases, the maximum pressure
 264 for the hot wall cases are higher than those for cold wall cases. This also
 265 leads to a relatively thinner flame when it impinges on the wall. This trend
 266 is observed for both fuels (see Figs. 6c and 6d).

267 Low temperature heat release (LTHR), which is observed for large hy-
 268 drocarbon flames under high pressure conditions, occurs between the wall
 269 and the flame front which is the location of the maximum heat release rate.
 270 Although this increases the unburned temperature by approximately 100 K,
 271 which can be seen in Figs. 6c and 6d, it does not seem to have significant
 272 effects on the wall heat flux induced by temperature differences between the
 273 preheated temperature of the fuel mixture and the wall as shown in Fig. 4b.
 274 The peak and burned-gas-induced heat flux still seem to be dominant. Note
 275 that according to the study by Popp et al. [6], including the Soret effect or
 276 surface reaction at wall temperatures larger than 400K affects the maximum
 277 wall heat flux, and decreases the discrepancies between experimental and
 278 numerical results. However, in their results, although the maximum value of
 279 wall heat flux is overestimated by about 10-20% without the Soret effect or
 280 surface reaction, the general trend of wall heat flux with wall temperature is

not influenced. Therefore, exclusion of the Soret effect and surface reaction does not unduly change the conclusion of the present study.

The wall temperature seems to significantly affect the quenching distance. Figure 7 shows the temporal developments of distance between wall and flames for cases of $P_{ini} = 10$ atm (M20W045) and $P_{ini} = 20$ atm (M20W045P). The wall temperature, EGR ratio and equivalence ratio are fixed at 450 K, 20% and 0.5, respectively to see the effects of chamber pressure on the quenching distance. Here, the flame position is identified as the location of the maximum heat release rate. The minimum value indicates the quenching distance, q_d , which decreases from 0.17 mm to 0.11 mm when the pressure is doubled. As shown in Fig. 7, this quenching distance may be measurable in scalar measurements since the trend is fully reproducible by using $[\text{CH}_2\text{O}] \times [\text{OH}]$ product [24, 25]. The quenching distances and peak Φ_q of all cases are summarized in Table 2. It can be seen that the wall temperature has a higher impact on the quenching distance than pressure change in the domain and clearly the peak Φ_q is dependent on the quenching distance.

The maximum Φ_q for all cases are normalized using the laminar flame power ($\Phi_f = \rho_{u,0} c_{p,u,0} (T_b - T_u) S_{L,0}$) obtained from the initial flame conditions, where ρ and c_p denote the density and specific heat at constant pressure, respectively. The subscript u and b indicate the unburned and burned sides, respectively. The normalized maximum wall heat flux, ($\Phi_n = \Phi_{q,max} / \Phi_f$), are shown in Table 2. Normalization by Φ_f , is used in many previous studies under constant pressure conditions [5–8, 26, 27]. Popp et al. [6] showed that the maximum Φ_n for a stoichiometric methane flame at atmospheric pressure is about 0.75 for chemically inactive wall boundaries and no Soret

306 effect. This value is very close to the present methane flames at a wall
 307 temperature of 450K, under different pressures, equivalence ratios and EGR
 308 ratios (M20W045P, M20W045, M20W045E, M10W045 & M15W045). In
 309 Table 2, the normalized maximum wall heat flux decreases with **increasing**
 310 mean pressure (M20W045 & M20W045P) and equivalence ratio (M20W045
 311 & M20W045E), **while** Φ_n increases with an increase of wall temperature.
 312 **Similar trends have** been reported in previous studies for non-EGR and con-
 313 stant pressure cases [5–8, 23, 26, 27], and clearly the present results show that
 314 this can be extended to isochoric and diluted conditions. This, together with
 315 the flame marker (pixel by pixel multiplication of mole fractions of CH₂O
 316 and OH) shown in Fig. 7, can be used in experimental studies to further our
 317 understanding of underlying physics of wall heat loss.

318 4. Conclusions

319 In this study, one-dimensional DNS of lean methane–air and *n*-heptane–
 320 air premixed flames with high EGR ratios propagating towards isothermal
 321 and inert walls in a head-on quenching configuration are conducted under
 322 **an** isochoric process to investigate wall heat flux and quenching distance
 323 at elevated pressure conditions. The effects of EGR ratio, equivalence ratio,
 324 initial pressure and wall temperature on flame–wall interaction are examined.

325 **Increased EGR ratios result** in reduced maximum wall heat flux and
 326 burned-gas-induced wall heat flux. It **was** found that **changes in** the equiv-
 327 alence ratio of the fuel mixture **have a** higher impact on the maximum wall
 328 heat flux than **changes in the** EGR ratio. Thus, leaner and more diluted
 329 combustion conditions are desirable on the heat loss point of view. The

330 flame-wall interaction time, $\tau_{fw}/\tau_{F,0}$, is not influenced by changing the EGR
331 ratio, equivalence ratio and initial chamber pressure for methane-air and n -
332 heptane-air flames at fixed wall temperature conditions. The dimensional
333 flame-wall interaction time is almost constant when the chamber pressure is
334 doubled. The influence of the low temperature oxidation in n -heptane flames
335 on wall heat flux induced by temperature differences between the preheated
336 temperature of the fuel mixture and the wall was found to be insignificant.
337 It was also shown that the thermal conductivity near the wall, as well as
338 the quenching distance, are sensitive to the wall temperature, and have a
339 substantial influence on the wall heat flux.

340 The present results also show that the findings in previous studies [5–8, 23,
341 26, 27] can be applied in a straightforward manner even for heat loss phe-
342 nomenon under pressure-varying conditions with/without low-temperature
343 chemistry in a range of ϕ , γ , P_{ini} and T_{wall} . Effects of turbulent motion on
344 heat loss characteristics will be investigated in future research.

345 Acknowledgments

346 This work was partly supported by Council for Science, Technology and
347 Innovation(CSTI), Cross-ministerial Strategic Innovation Promotion Program
348 (SIP), Innovative Combustion Technology (Funding agency: JST).

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Table 1: Numerical parameters for DNS of methane–air and *n*-heptane–air premixed flames.

Methane & <i>n</i> -Heptane	ϕ	γ [%]	$S_{L,0}$ [m/s]	$\delta_{th,0}$ [mm]	T_{wall} [K]	P_{ini} [atm]	$T_{ad,0}$ [K]
M10W045	0.5	10	0.137	0.208	450	10	1743
M15W045	0.5	15	0.119	0.236	450	10	1713
M20W045	0.5	20	0.102	0.270	450	10	1680
M20W045E	0.6	20	0.166	0.175	450	10	1816
M20W070	0.5	20	0.102	0.270	700	10	1680
M20W090	0.5	20	0.102	0.270	900	10	1680
M20W110	0.5	20	0.102	0.270	1100	10	1680
M20W045P	0.5	20	0.075	0.188	450	20	1680
H20W045	0.5	20	0.156	0.188	450	10	1711
H20W070	0.5	20	0.156	0.188	700	10	1711
H20W090	0.5	20	0.156	0.188	900	10	1711

Table 2: Quenching distance, $\Phi_{q,max}$ and Φ_n .

	q_d [mm]	$\Phi_{q,max}$ [MW/m ²]	Φ_n
M10W045	0.130	0.601	0.741
M15W045	0.148	0.517	0.754
M20W045	0.169	0.438	0.770
M20W045E	0.106	0.801	0.754
M20W070	0.101	0.713	1.254
M20W090	0.059	1.283	2.255
M20W110	0.026	2.641	4.644
M20W045P	0.114	0.625	0.747
H20W045	0.071	0.497	0.535
H20W070	0.038	0.789	0.849
H20W090	0.022	1.296	1.394

Figure 1: Schematic of the computational domain (a) and initial temperature distribution in the domain (b). Wall boundary at $x = -2.5$ and 2.5 mm. Arrows indicate the direction of flame propagation after ignition.

Figure 2: Temporal developments of mean pressure and wall heat flux of methane flames with different EGR ratio.

Figure 3: Temporal developments of wall heat flux of methane flames at different equivalence ratio (a) and at different initial pressure conditions with mean pressure (b).

Figure 4: Temporal developments of wall heat flux at different wall temperature conditions for methane-air (a) and *n*-heptane-air (b) flames.

Figure 5: Maximum wall heat flux and thermal conductivity of methane (red open symbols) and *n*-heptane (black closed symbols) as a function of wall temperature.

Figure 6: Temporal developments of temperature for methane-air and n -heptane-air flames at different wall temperature conditions. (a,b): methane-air flames. (c,d): n -heptane-air flames.

Figure 7: Distance from wall for methane flames.

Nomenclature

γ	EGR ratio
ϕ	Equivalence ratio
T_{wall}	Wall temperature
T	Temperature
T_u	Unburned temperature
T_b	Burned temperature
T_{wall}	Wall temperature
T_{pre}	Preheated temperature
T_{ini}	Initial temperature distribution
T_{max}	Maximum temperature
$T_{ad,0}$	Adiabatic flame temperature
P_{ini}	Initial chamber pressure
r_c	Radius of the ignition kernel
σ_T	The distance from center to the position at which the temperature gradient is maximum
Φ_q	Wall heat flux
Φ_n	Normalized maximum wall heat flux
Φ_f	Laminar flame power
$\delta_{th,0}$	Thermal flame thickness at initial pressure conditions
$S_{L,0}$	Laminar burning velocity at initial pressure conditions
ϕ	Equivalence ratio
ρ	Density
$\mathbf{u}$	Fluid velocity vector

λ	Thermal conductivity of the gaseous mixture
N_s	Number of chemical species
Y_i	Mass fraction for species i
$\mathbf{V}_i$	Diffusion velocity for chemical species i
R_i	Characteristic gas constant for chemical species i
h_i	Enthalpy for chemical species i
w_i	Reaction rate for chemical species i
$c_{v,i}$	Heat capacity at constant volume for chemical species i
$c_{p,i}$	Heat capacity at constant pressure for chemical species i
$\bar{c}_v$	Mixture averaged specific heat capacity at constant volume
$\mathbf{P}$	Stress tensor
p	Pressure
μ	Dynamic viscosity
$\tau_{F,0}$	Flame time at initial pressure conditions
τ_{fw}	Flame–wall interaction time